

4-Bromo-5-methoxy-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)thiophene-2-carboxamide
113589-05-2 | DTXSID60556730

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.66

Global applicability domain: Inside

Local applicability domain index: 3.83e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Bromo-5-methoxy-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)thiophene-2-carboxamide

Measured: 1.35

Predicted: 1.66

[Image not found](#)

4,5-Dibromo-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)thiophene-2-carboxamide

Measured: 1.85

Predicted: 1.83